

## In Vivo and In Vitro Data Comparison of Ocular Irritancy Classification: Sorted by Reference

Substance/Product Name	CASRN <sup>1</sup>	Concentration Tested	Overall <i>In Vivo</i> Classification (GHS)	<i>In Vitro</i> Classification (GHS)	<i>In Vivo</i> Classification (GHS) <sup>2,3</sup>	Overall <i>In Vivo</i> Classification (EPA)	<i>In Vitro</i> Classification (EPA)	<i>In Vivo</i> Classification (EPA) <sup>4,5</sup>	Overall <i>In Vivo</i> Classification (EU)	<i>In Vitro</i> Classification (EU)	<i>In Vivo</i> Classification (EU) <sup>6,7</sup>	FHSA-20% <sup>8</sup>	FHSA-67% <sup>9</sup>	Reference
1-Naphthaleneacetic acid	86-87-3	neat	1	2B	1	I	III	I	R41	R36	SCNM	Irritant	Irritant	Balls et al. (1995)
1-Naphthaleneacetic acid, sodium salt	61-31-4	neat	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	undiluted	2B	2A	2A	II	II	II	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	undiluted	1	1	SCNM <sup>10</sup>	I	I	I	R41	R41	SCNM	Irritant	Irritant	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	neat	1	2B	1	I	III	I	R41	R36	R41	Irritant	Irritant	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	undiluted	2A	2A	2A	II	II	II	R36	R36	SCNM	Irritant	Irritant	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	neat	2A	NI	2A	II	IV	II	R36	NI	R36	Irritant	Irritant	Balls et al. (1995)
Acetone	67-64-1	undiluted	2A	2A	2A	II	II	II	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
Ammonium nitrate	6484-52-2	undiluted	2B	2B	2B	III	III	III	R36	NI	R36	Irritant	Irritant	Balls et al. (1995)
Benzalkonium chloride (1%)	8001-54-5	1%	1	2A	1	I	II	I	R41	R36	R41	Irritant	Irritant	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	10%	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	5%	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Captan 90 concentrate	133-06-2	neat	1	2B	1	I	III	I	R41	NI	R41	Irritant	Irritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	0.1%	NI	2B	NI	III	III	III	NI	NI	NI	Irritant	Inconclusive	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	10%	1	2A	1	I	II	I	R41	R36	R41	Irritant	Irritant	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	6%	1	2A	1	SCNM	II	SCNM	R41	R36	R41	Irritant	Irritant	Balls et al. (1995)
Chlorhexidine	55-56-1	neat	1	1	1	I	I	SCNM	R41	R41	SCNM	Irritant	Irritant	Balls et al. (1995)
Cyclohexanol	108-93-0	undiluted	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	neat	1	1	1	SCNM	I	SCNM	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	neat	2A	2A/2B	2A	II	II/III	II	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
Ethanol	64-17-5	undiluted	2B	1	2A	III	I	III	NI	R41	NI	Irritant	Irritant	Balls et al. (1995)
Ethyl acetate	141-78-6	undiluted	NI	2A	NI	III	II	III	NI	R36	NI	Irritant	Irritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	undiluted	NI	2B	NI	III	III	III	NI	NI	NI	Not Labeled	Not Labeled	Balls et al. (1995)
Ethyl-2-methylacetacetate	609-14-3	undiluted	2B	2B	III	III	III	III	NI	NI	NI	Irritant	Irritant	Balls et al. (1995)
Fomesafen	72128-02-0	neat	NI	2B	NI	III	III	III	NI	NI	NI	Irritant	Irritant	Balls et al. (1995)
Gammabutyrolactone	96-48-0	undiluted	2B	2A	2A	II	II	II	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
Glycerol	56-81-5	undiluted	NI	2B	NI	IV	III	IV	NI	NI	NI	Not Labeled	Not Labeled	Balls et al. (1995)
Imidazole	288-32-4	neat	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Isobutanol	78-83-1	undiluted	2B	1	2A	II	I	II	R36	R41	R36	Irritant	Irritant	Balls et al. (1995)
Isopropanol	67-63-0	undiluted	2B	1	2A	III	I	III	R36	R41	SCNM	Irritant	Irritant	Balls et al. (1995)
L-Aspartic acid	70-47-3	neat	SCNM	2A	SCNM	SCNM	II	SCNM	R36	R36	SCNM	Irritant	Irritant	Balls et al. (1995)
Maneb	12427-38-2	neat	2B	NI	SCNM	III	IV	III	R36	NI	SCNM	Irritant	Irritant	Balls et al. (1995)
Methyl acetate	79-20-9	undiluted	2B	1	2A	II	I	II	R36	R41	R36	Irritant	Irritant	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	undiluted	2A	NI	2A	II	IV	II	R36	NI	R36	Irritant	Irritant	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	undiluted	2B	1	2A	III	I	III	R36	R41	R36	Irritant	Irritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	undiluted	NI	2A	NI	III	II	III	NI	R36	NI	Irritant	Inconclusive	Balls et al. (1995)
Methylcyclopentane	96-37-7	undiluted	NI	NI	NI	III	IV	III	NI	NI	NI	Not Labeled	Not Labeled	Balls et al. (1995)
n-Butyl acetate	123-86-4	undiluted	NI	2A	NI	III	II	III	NI	R36	NI	Irritant	Inconclusive	Balls et al. (1995)
n-Hexanol	111-27-3	undiluted	2A	1	2A	II	I	II	R36	R41	R36	Irritant	Irritant	Balls et al. (1995)
n-Octanol	111-87-5	undiluted	2B	2A	2B	II	II	II	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
Parafluoraniline	371-40-4	undiluted	SCNM	1	SCNM	SCNM	I	SCNM	R36	R41	SCNM	Irritant	Irritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	undiluted	NI	2B	NI	IV	III	IV	NI	R36	NI	Not Labeled	Not Labeled	Balls et al. (1995)
Potassium cyanate	590-28-3	neat	SCNM	2B	SCNM	SCNM	III	SCNM	R36	R36	SCNM	Irritant	Irritant	Balls et al. (1995)
Promethazine HCl	58-33-3	neat	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Pyridine	110-86-1	undiluted	1	1	1	I	I	I	R41	R41	R41	Irritant	Irritant	Balls et al. (1995)
Quinacrine	69-05-6	neat	1	2B	1	I	III	I	R41	NI	R41	Irritant	Irritant	Balls et al. (1995)
Sodium hydroxide (1%)	1310-73-2	1%	2B	2A	2B	III	II	III	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	10%	1	1	1	I	I	I	R41	R41	R41	scnm	scnm	Balls et al. (1995)
Sodium lauryl sulfate (15%)	151-21-3	15%	1	2B	1	I	III	I	R36	R36	R36	Irritant	Irritant	Balls et al. (1995)
Sodium lauryl sulfate (3%)	151-21-3	3%	NI	2B	NI	III	III	III	NI	NI	NI	Irritant	Irritant	Balls et al. (1995)
Sodium oxalate	62-76-0	neat	1	2B	1	I	III	I	R41	NI	R41	Irritant	Irritant	Balls et al. (1995)

## In Vivo and In Vitro Data Comparison of Ocular Irritancy Classification: Sorted by Reference

Substance/Product Name	CASRN <sup>1</sup>	Concentration Tested	Overall In Vivo Classification (GHS)	In Vitro Classification (GHS) <sup>2,3</sup>	In Vivo Classification (GHS) <sup>2,3</sup>	Overall In Vivo Classification (EPA)	In Vitro Classification (EPA)	In Vivo Classification (EPA) <sup>4,5</sup>	Overall In Vivo Classification (EU)	In Vitro Classification (EU)	In Vivo Classification (EU)	FHSA-20% <sup>8</sup>	FHSA-67% <sup>9</sup>	Reference
Sodium perborate, 4H <sub>2</sub> O	10486-00-7	neat	I	2B	1	I	III	I	R41	NI	R41	Irritant	Irritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	neat	NI	2B	NI	III	III	III	NI	NI	NI	Irritant	Irritant	Balls et al. (1995)
Toluene	108-88-3	undiluted	NI	2A	NI	III	II	III	NI	R36	NI	Irritant	Irritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	3%	NI	2A	NI	III	II	III	NI	R36	NI	Irritant	Inconclusive	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	30%	I	I	I	I	I	I	R41	R41	R41	scnm	scnm	Balls et al. (1995)
Triton X-100 (10%)	9002-93-1	10%	2A	2A/2B	1	II	II/III	II	R36	R36	R41	Irritant	Irritant	Balls et al. (1995)
Triton X-100 (5%)	9002-93-1	5%	2B	2A	2A	III	II	III	R36	R36	NI	Irritant	Irritant	Balls et al. (1995)
Tween 20	9005-64-5	undiluted	NI	2B	NI	III	III	III	NI	NI	NI	Irritant	Inconclusive	Balls et al. (1995)
TNO-01 (Formulation-1)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-02 (Formulation-2)	n.p.	undiluted			2A	2A	II	II		R36	R36	Irritant	Irritant	Prinsen (1996)
TNO-03 (Pesticide-1)	n.p.	undiluted			NI	NI	IV	III		NI	NI	Irritant	Irritant	Prinsen (1996)
TNO-04 (Detergent-1)	n.p.	undiluted			2B	2A	III	III		NI	NI	Irritant	Irritant	Prinsen (1996)
TNO-05 (Silicone powder-1)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-06 (Lubricant)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-07 (Ink-1)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-08 (Ink-2)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-09 (Paint)	n.p.	undiluted			NI	NI	IV	II		NI	NI	Irritant	Irritant	Prinsen (1996)
TNO-10 (Silicone powder-2)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-11 (Sodium p-styrene sulfonate)	2695-37-6	undiluted			2A	SCNM	II	SCNM		R36	SCNM	Irritant	Irritant	Prinsen (1996)
TNO-12 (Formulation-3)	n.p.	undiluted			2A	NI	II	SCNM		R36	R36	Irritant	Irritant	Prinsen (1996)
TNO-13 (Pesticide-2)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-14 (Polydisaccharide)	n.p.	14.5%			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-15 (Polydisaccharide)	n.p.	50%			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-16 (Liquid nylon product)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-17 (Solvent-1)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-18 (Solvent-2)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-19 (Solvent-3)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-20 (Solvent-4)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-21 (Solvent-5)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-22 (Solvent-6)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-23 (Solvent-7)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-24 (Solvent-8)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-25 (Solvent-9)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-26 (Ink-3)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-27 (Thermal paper coating-1)	n.p.	undiluted			2B	2B	III	III		NI	NI	Irritant	Irritant	Prinsen (1996)
TNO-28 (Toilet cleaner-1)	n.p.	undiluted			2B	I	III	I		NI	R41	Irritant	Irritant	Prinsen (1996)
TNO-29 (Toilet cleaner-2)	n.p.	undiluted			2B	2A	III	III		NI	R36	Irritant	Irritant	Prinsen (1996)
TNO-30 (Pesticide-3)	n.p.	undiluted			2B	NI	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-31 (Sulfur)	7704-34-9	undiluted			NI	NI	IV	III		NI	NI	Irritant	Inconclusive	Prinsen (1996)
TNO-32 (Ink-4)	n.p.	undiluted			2B	NI	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-33 (Thermal paper coating-2)	n.p.	undiluted			2B	NI	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-34 (Detergent-2)	n.p.	undiluted			I	SCNM	I	SCNM		R41	SCNM	Irritant	Irritant	Prinsen (1996)
TNO-35 (Propyl-lactate)	616-09-1	undiluted			I	I	I	I		R41	R41	scnm	scnm	Prinsen (1996)
TNO-36 (Ethylhexyl lactate)	6283-86-9	undiluted			2A	SCNM	II	II		R36	SCNM	Irritant	Irritant	Prinsen (1996)
TNO-37 (Pesticide-4)	n.p.	undiluted			2B	2B	III	III		NI	NI	Irritant	Irritant	Prinsen (1996)
TNO-38 (Solvent-10)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-39 (Detergent-3)	n.p.	undiluted			NI	NI	IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (1996)
TNO-40 (Glycolbromoacetate form.)	n.p.	undiluted			I	-	I	-		R41	R41 (SC)			Prinsen (1996)
TNO-41 (Amidosulfonic acid)	5329-14-6	undiluted			I	-	I	-		R41	R41 (SC)			Prinsen (1996)
TNO-42 (Glycolbromoacetate)	3785-34-0	85%			I	-	I	-		R41	R41 (SC)			Prinsen (1996)
TNO-43 (Monobromoacetic acid)	79-08-3	undiluted			I	-	I	-		R41	R41 (SC)			Prinsen (1996)

### In Vivo and In Vitro Data Comparison of Ocular Irritancy Classification: Sorted by Reference

Substance/Product Name	CASRN <sup>1</sup>	Concentration Tested	Overall <i>In Vivo</i> Classification (GHS)	<i>In Vitro</i> Classification (GHS) <sup>2,3</sup>	<i>In Vivo</i> Classification (GHS) <sup>2,3</sup>	Overall <i>In Vivo</i> Classification (EPA)	<i>In Vitro</i> Classification (EPA)	<i>In Vivo</i> Classification (EPA) <sup>4,5</sup>	Overall <i>In Vivo</i> Classification (EU)	<i>In Vitro</i> Classification (EU)	<i>In Vivo</i> Classification (EU) <sup>6,7</sup>	FHSA-20% <sup>8</sup>	FHSA-67% <sup>9</sup>	Reference
TNO-44 (Didecyldimethylammoniumchloride (23% in propyl glycol))	7173-51-5	23%		1	-		I	-		R41	R41 (SC)			Prinsen (1996)
Cetylpyridinium bromide (6%)	—	undiluted	R41	1	1		I	SCNM	I	R41	R41	Irritant	Irritant	Prinsen (2000)
cyclohexylamino-functional PMS	—	undiluted	R36	2A	-		II	-	II	R36	R36			Prinsen (2000)
decamethylcyclopentasiloxane	—	undiluted	NI	NI	-		NI	-	NI	NI	NI			Prinsen (2000)
Triton X-500 (5%)	—	undiluted	NI	2B	-		III	-	III	NI	R36			Prinsen (2000)
TNO-45	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-46	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-47	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-48	n.p.	undiluted		2A	-	2A	II	-		R36	R41 (SC)			Prinsen (2005)
TNO-49	n.p.	undiluted		1	-	1	I	-		R41	R41 (SC)			Prinsen (2005)
TNO-50	n.p.	undiluted		1	-	1	I	-		R41	R41 (SC)			Prinsen (2005)
TNO-51	n.p.	undiluted		1	-	1	I	-		R41	R41 (SC)			Prinsen (2005)
TNO-52	n.p.	undiluted		2B	2A	2B	III	III		NI	R36	Irritant	Irritant	Prinsen (2005)
TNO-53	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-54	n.p.	undiluted		2B	2B	2B	III	III		NI	NI	Irritant	Irritant	Prinsen (2005)
TNO-55	n.p.	undiluted		2B	2A	2B	III	III		R36	R36	Irritant	Irritant	Prinsen (2005)
TNO-56	n.p.	undiluted		2B	2B	2B	III	III		R36	NI	Irritant	Irritant	Prinsen (2005)
TNO-57	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-58	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-59	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-60	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-61	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-62	n.p.	undiluted		2B	NI	2B	III	III		R36	NI	Irritant	Irritant	Prinsen (2005)
TNO-63	n.p.	undiluted		NI	NI	NI	NI	IV	III	NI	NI	Irritant	Irritant	Prinsen (2005)
TNO-64	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-65	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-66	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-67	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-68	n.p.	undiluted		2A	2A	2A	II	II		R36	R36	Irritant	Irritant	Prinsen (2005)
TNO-69	n.p.	50%		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-70	n.p.	undiluted		2A	2A	2A	II	III		R36	R36	Irritant	Irritant	Prinsen (2005)
TNO-71	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-72	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-73	n.p.	undiluted		1	2A	1 (LE)	I	II		R41	R36	Irritant	Irritant	Prinsen (2005)
TNO-74	n.p.	undiluted		NI	NI	NI	NI	IV	III	NI	NI	Irritant	Inconclusive	Prinsen (2005)
TNO-75	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-76	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-77	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-78	n.p.	undiluted		2B	2B	2B	III	III		NI	NI	Irritant	Irritant	Prinsen (2005)
TNO-79	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-80	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-81	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-82	n.p.	undiluted		NI	NI	NI	NI	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-83	n.p.	undiluted		2B	2B	2B	III	III		NI	R36	Irritant	Irritant	Prinsen (2005)
TNO-84	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-85	n.p.	undiluted		2B	1	2B	III	I		R36	R41	Irritant	Irritant	Prinsen (2005)
TNO-86	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)

## In Vivo and In Vitro Data Comparison of Ocular Irritancy Classification: Sorted by Reference

Substance/Product Name	CASRN <sup>1</sup>	Concentration Tested	Overall In Vivo Classification (GHS)	In Vitro Classification (GHS) <sup>2,3</sup>	In Vivo Classification (GHS) <sup>2,3</sup>	Overall In Vivo Classification (EPA)	In Vitro Classification (EPA) <sup>4,5</sup>	In Vivo Classification (EPA) <sup>4,5</sup>	Overall In Vivo Classification (EU)	In Vitro Classification (EU)	In Vivo Classification (EU) <sup>6,7</sup>	FHSA-20% <sup>8</sup>	FHSA-67% <sup>9</sup>	Reference
TNO-87	n.p.	undiluted		2B	NI	2B	III	IV		NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-88	n.p.	undiluted		NI	NI	NI	IV			NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-89	n.p.	undiluted		NI	NI	NI	IV			NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-90	n.p.	undiluted		NI	NI	NI	IV			NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-91	n.p.	undiluted		NI	NI	NI	IV			NI	NI	Not Labeled	Not Labeled	Prinsen (2005)
TNO-92	n.p.	undiluted		2B	1	2B	III	I		R36	R41	scnm	scnm	Prinsen (2005)
TNO-93	n.p.	undiluted		2A	1	2A	II	I		R36	R41	scnm	scnm	Prinsen (2005)
TNO-94	n.p.	undiluted		NI	1	NI	NI	I		NI	R41	Irritant	Irritant	Prinsen (2005)
1-Butanol	71-36-3	undiluted		1	2A		I	II		R41	R41	Irritant	Irritant	Prinsen and Koeter (1993)
2-Butoxyethyl acetate	112-07-2	undiluted		2B	-		III	-		NI	NI			Prinsen and Koeter (1993)
2-Methoxyethanol	109-86-4	undiluted		2A	-		II	-		R36	R36	Irritant	Irritant	Prinsen and Koeter (1993)
Acetaldehyde	75-07-0	undiluted		2A	-		II	-		R36	R36	Irritant	Irritant	Prinsen and Koeter (1993)
Acetic acid	64-19-7	10%		1	1		I	I		R41	R41	Irritant	Irritant	Prinsen and Koeter (1993)
Benzalkonium chloride (100%)	8001-54-5	undiluted		1	1		I	I		R41	R41	Irritant	Irritant	Prinsen and Koeter (1993)
Brij 35	9002-92-0	undiluted		NI	-		IV	-		NI	NI	Not Labeled	Not Labeled	Prinsen and Koeter (1993)
Chloroform	67-66-3	undiluted		2A	-		II	-		R36	R36			Prinsen and Koeter (1993)
Dibutyltin dichloride	683-18-1	undiluted		1	-		I	-		R41	R41			Prinsen and Koeter (1993)
Dimethyl sulfoxide	67-68-5	undiluted		NI	2B		IV	III		NI	NI	Irritant	Inconclusive	Prinsen and Koeter (1993)
Glycerol	56-81-5	undiluted		NI	NI		IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen and Koeter (1993)
Mercury (II) chloride	7487-94-7	undiluted		1	-		I	-		R41	R41			Prinsen and Koeter (1993)
n-Hexane	110-54-3	undiluted		NI	NI		IV	IV		NI	NI	Not Labeled	Not Labeled	Prinsen and Koeter (1993)
Silver (I) nitrate	7761-88-8	3%		2B	-		III	-		NI	NI			Prinsen and Koeter (1993)
Sodium dodecyl sulfate	151-21-3	undiluted		2B	-		III	-		R41	R41			Prinsen and Koeter (1993)
Sodium fluorescein	518-47-8	20%		NI	-		IV	-		NI	NI			Prinsen and Koeter (1993)
Sodium hydroxide	1310-73-2	1%		1	1		I	I		R41	R41			Prinsen and Koeter (1993)
Toluene	108-88-3	undiluted		2B	2B		III	III		NI	NI			Prinsen and Koeter (1993)
Triacetin	102-76-1	undiluted		NI	NI		IV	IV		NI	NI			Prinsen and Koeter (1993)
Tributyltin chloride	1461-22-9	undiluted		1	-		I	-		R41	R41			Prinsen and Koeter (1993)
Triethanolamine	102-71-6	undiluted		2B	NI		III	III		NI	NI	Not Labeled	Not Labeled	Prinsen and Koeter (1993)

<sup>1</sup>CASRN=Chemical Abstract Services Registry Number

<sup>2</sup>GHS=Globally Harmonized System (UN 2007)

<sup>3</sup>Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant.

<sup>4</sup>NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance: 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are both severe and persistent; and 4: corneal opacity score equal to 4 at any time; NC: not classified because none of the above criteria were met

<sup>4</sup>EPA=U.S. Environmental Protection Agency (EPA 2003a).

<sup>5</sup>Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 1-7 days; Category IV: minimal effects clearing in less than 24 hr

<sup>6</sup>EU=European Union (EU 2001).

<sup>7</sup>Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; NI = not an eye irritant.

<sup>8</sup>FHSA=Federal Hazardous Substance Act (2005). FHSA-20% is based on the proportion of positive animals needed to identify a substance as an irritant using the FHSA sequential testing strategy, where 20% of the animals need to demonstrate a positive response for a substance to be identified as an irritant. A substance tested using 3 to 6 animals would not be labeled if ≤ 1/6 animals were positive based on the FHSA criteria. The substance would be labeled as an irritant if there were ≥1 positive animal in a 3 to 5 animal test or >2 positive animals in a 6 animal test

<sup>9</sup>FHSA=Federal Hazardous Substances Act (2005). FHSA-67% is based on the proportion of positive animals needed to identify a substance as an irritant using the "first test" of the FHSA sequential testing strategy, where 67% of the animals need to demonstrate a positive response for a substance to be identified as an irritant. A substance tested using 3 to 6 animals would not be labeled if ≤ 1/6 animals were positive based on the FHSA criteria. The substance would be labeled as an irritant if there were >2/3, 3/4, 4/5, or 4/6 positive animals. If 1/3, 1/4, 2/4, 1/5, 2/5, 3/5, 2/6, or 3/6 animals were positive, further testing would be required.

<sup>10</sup>SCNM = study criteria not met